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ABSTRACT

Compound-specific diffusivities significantly impact solute transport and mixing at different scales. Although diffusive processes occur at the small pore scale, their effects propagate and remain important at larger macroscopic scales [1]. In this pore-scale modeling study in saturated porous media we show that compound-specific effects are important not only at steady-state and for the lateral displacement of solutes with different diffusivities but also for transient transport and solute breakthrough [2]. We performed flow and transport simulations in two-dimensional pore-scale domains with different arrangement of the solid grains leading to distinct characteristics of flow variability and connectivity, representing mildly and highly heterogeneous porous media, respectively. The results obtained for a range of average velocities representative of groundwater flow (0.1–10 m/day), show significant effects of aqueous diffusion on solute breakthrough curves. However, the magnitude of such effects can be masked by the flux-averaging approach used to measure solute breakthrough and can hinder the correct interpretation of the true dilution of different solutes. We propose, as a metric of mixing, a transient flux-related dilution index that allows quantifying the evolution of solute dilution at a given position along the main flow direction. For the different solute transport scenarios we obtained dilution breakthrough curves that complement and add important information to traditional solute breakthrough curves. Such dilution breakthrough curves allow capturing the compound-specific mixing of the different solutes and provide useful insights on the interplay between advective and diffusive processes, mass transfer limitations, and incomplete mixing in the heterogeneous pore-scale domains. The quantification of dilution for conservative solutes is in good agreement with the outcomes of mixing-controlled reactive transport simulations, in which the mass and concentration breakthrough curves of the product of an instantaneous transformation of two initially segregated reactants were used as measures of reactive mixing.

REFERENCES

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